RKKY interaction in the nearly-nested Fermi liquid

D.N. Aristov [1,2], S.V. Maleyev [2]

[1] *Laboratoire Léon Brillouin, CE-Saclay, 91191 Gif-sur-Yvette Cedex, France.*
[2] *Petersburg Nuclear Physics Institute, Gatchina, St. Petersburg 188350, Russia*

(February 1, 2008)

We present the results of analytical evaluation of the indirect RKKY interaction in a layered metal with nearly nested (almost squared) Fermi surface. The final expressions are obtained in closed form as a combination of Bessel functions. We discuss the notion of the "$2k_F$" oscillations and show that they occur as the far asymptote of our expressions. We show the existence of the intermediate asymptote of the interaction which is of the sign-reversal antiferromagnetic type and is the only term surviving in the limit of exact nesting. A good accordance of our analytical formulas with numerical findings is demonstrated until the interatomic distances. The obtained expressions for the Green's functions extend the previous analytical results into the region of intermediate distances as well.

75.30.Et, 74.72.-h, 75.20.Hr

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction was found to play an important role in various problems involving the interaction of localized moments in a metal via polarization of conduction electrons. The spatial dependence of this interaction for the spherical Fermi surface (FS) in three dimensions was obtained in Ref.[1] about 40 years ago. It was demostrated there that at large distances r the interaction decays as r^{-3} and has the $2k_F$ oscillations with the Fermi momentum k_F. Later Roth, Zeiger and Kaplan[2] have generalized this result for the case of non-spherical FS. The interaction was represented as a series in $1/r$ and the existence of the direction-dependent period of oscillations $(2k_F^*)^{-1}$ was shown.

The limitation of this latter result is the inapplicability of the theory at small distances $k_F^* r \lesssim 1$, i.e. in the region where the RKKY interaction is mostly significant. It could be among the plausible reasons for the nowaday situation, when the notion of $2k_F$ oscillations is widely explored while the actual meaning of this term for the non-spherical FS remains unclear in many cases. Numerical calculations are instrumental[3] to extend our understanding of non-spherical FS ever since 1957, but a theoretical understanding even on a qualitative level is very important.

In a recent paper one of the authors presented the method which enabled to obtain in a simple manner the RKKY interaction for the spherical FS and any dimensionality of the system. The closed expressions were found both in $r-$ and $q-$ representations.[4]

In the present paper we generalize this method to arrive to the closed analytical expressions for the RKKY interaction in a layered (2D) metal with highly non-spherical (nearly nested) Fermi surface. Our main results could be summarized as follows.
i) The RKKY interaction for this type of the FS consists of three parts. The first one stems from the flat regions in the fermionic spectrum. This term decays mostly as $1/r$ and is important only along the diagonals $x = \pm y$ in the **r**−space.
ii) The second part of the RKKY interaction is contributed by the vicinities of the points $(0, \pi)$ and $(\pi, 0)$.

These are the saddle points in the fermionic dispersion giving rise to the van Hove singularities. At $r \to \infty$ this part of RKKY takes its exact correspondence with the previous findings.[2] It turns out however that it is the far asymptote of the interaction.
iii) At $k_F^* r \lesssim 1$ the third part of the interaction comes into play. This intermediate asymptote arises as an interference between contributions from the vicinities of the different van Hove points. This term possesses the overall prefactor $\cos(\mathbf{Q}\mathbf{r})$ with the spanning wave-vector $\mathbf{Q} = (\pi, \pi)$. In the nearly nested situation this last term is present down to the interatomic distances and strongly favors the commensurate antiferromagnetic ordering of the localized moments.
iv) The last but not least. We show both analytically and numerically that our expressions are valid near the interatomic distances. This result could be qualitatively explained in the following way. It is clear that to evaluate the interaction at the distances r one should know the details of the fermionic dispersion on a scale $1/r$ in **k**−space. Hence the finest details of the Fermi surface are of importance at the largest distances. One may also conclude that even rough knowledge of the spectrum over the whole Brillouin zone is enough for a good description of the corresponding quantities at the interatomic distances in **r**−space. This is exactly what our method does by grasping the key features of the FS.

The rest of the paper is organized as follows. We formulate the problem and introduce the basic ingredients of our treatment in Sections I and II. The Green's functions resulted from the van Hove points of the spectrum are found in Section III. Their contribution to the RKKY interaction is analyzed in Section IV. The role of the flat parts of the spectrum is discussed in Section V. We make the concluding remarks in the Section VI of the paper.

I. GENERAL FORMALISM

We begin with conventional form of the exchange interaction between the localized moment **J** and electron

spin density $\mathbf{s}(\mathbf{r})$:

$$V(\mathbf{r}) = -A\mathbf{J}(\mathbf{R})\mathbf{s}(\mathbf{r})\delta(\mathbf{R} - \mathbf{r}) \qquad (1)$$

Here A is the exchange coupling constant. The RKKY interaction between two localized moments via the conduction electrons may then be written in the following form

$$H_{RKKY} = -\frac{1}{2}A^2\mathbf{J}_1\mathbf{J}_2\chi(\mathbf{r}_1, \mathbf{r}_2) . \qquad (2)$$

where $r-$dependent part of the interaction coincides with the Fourier transform of the non-uniform static susceptibility $\chi(q)$ (Lindhard function) and is usually written in the form :

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = \frac{v_0^2}{(2\pi)^6}\int d^3\mathbf{k}\,d^3\mathbf{q}\,\frac{n_k - n_q}{\varepsilon_q - \varepsilon_k}e^{i(\mathbf{q}-\mathbf{k})(\mathbf{r}_1-\mathbf{r}_2)} \qquad (3)$$

with the unit cell volume v_0 and the Fermi function $n_k = (\exp(\varepsilon_k/T) + 1)^{-1}$. For our purpose, it is more convenient however to represent the above expression in the equivalent form

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = -T\sum_n G(i\omega_n, \mathbf{r}_1, \mathbf{r}_2)G(i\omega_n, \mathbf{r}_2, \mathbf{r}_1) \qquad (4)$$

here Matsubara frequency $\omega_n = \pi T(2n + 1)$ and G is the electronic Green's function. In the case of low temperatures considered below we use the limiting relation $T\sum_n \to \int_{-\infty}^{\infty} d\omega/(2\pi)$.

The electronic Green's function is given by

$$G(i\omega, \mathbf{r}_1, \mathbf{r}_2) = \frac{v_0}{(2\pi)^3}\int d^3\mathbf{k}\frac{\exp(i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2))}{i\omega - \varepsilon_k}u_k(\mathbf{r}_1)u_k^*(\mathbf{r}_2) \qquad (5)$$

with the periodic Bloch function $u_k(\mathbf{r})$. Generally speaking the $u-$functions should be inserted into (3), and it is the case of free electrons only when the RKKY interaction depends on the absolute value of the distance $\mathbf{r}_1 - \mathbf{r}_2$. We consider below the tight-binding form of the electronic Hamiltonian which implies the following form of $u_k(\mathbf{r})$[5]:

$$u_k(\mathbf{r}) = \sum_n e^{i\mathbf{k}(\mathbf{a}_n-\mathbf{r})}\varphi(\mathbf{r} - \mathbf{a}_n), \qquad (6)$$

here the Wannier function $\varphi(\mathbf{r})$ rapidly decays with distance and is close to the atomic wave-function at small $\mathbf{r}$. In view of this rapid decrease on the scale of interatomic distances, it is possible to neglect the dependence of $u_k(\mathbf{r})$ on $\mathbf{k}$ within the first Brillouin zone for most positions of $\mathbf{r}$ in the unit cell. Therefore we may replace $u_k(\mathbf{r})$ by $u_0(\mathbf{r})$ and assume the exchange coupling is appropriately redefined, $A \to A|u_0(\mathbf{r})|^2$. It is clear that upon this redefinition the Green's function (5) depends only on the difference $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$.

In view of forthcoming consideration we stress that the above replacement of the amplitude of Bloch function is the only uncontrolled appoximation of our treatment. The relevant calculations[6] show that $\varphi(\mathbf{r})$ for the nearest neighbors is of order of magnitude smaller than $\varphi(0)$. Therefore we expect that omitting the dependence of $u_k(\mathbf{r})$ on $\mathbf{k}$ might cause only minor corrections to our results.

II. NEARLY NESTED FERMI SURFACE

We consider a two-dimensional case of almost nested Fermi surface, with the quasiparticle dispersion given by

$$\varepsilon_\mathbf{k} = -2t(\cos k_x + \cos k_y) - \mu, \quad |\mu| \ll t \qquad (7)$$

with $t > 0$. This tight-binding form of the spectrum particularly appeared in different models related to the high-T_c phenomenon.[7] Henceforth we let the lattice parameter to be unity.

We will regard the different parts of the spectrum (7) on the different manner. We divide the whole FS onto four parts, which are as follows.

The vicinities of the saddle points of the spectrum. The dispersion near the points $(0, \pm\pi)$ and $(\pm\pi, 0)$ are given by

$$\varepsilon_{(0,\pm\pi)+\mathbf{k}} \simeq t(k_x^2 - k_y^2) - \mu + O(tk^4), \qquad (8)$$

$$\varepsilon_{(\pm\pi,0)+\mathbf{k}} \simeq -t(k_x^2 - k_y^2) - \mu + O(tk^4), \qquad (9)$$

respectively.

The flat parts of the Fermi surface. In the vicinity of the pair of wave-vectors $\pm(\pi/2, \pi/2)$ the dispersion takes the form similar to the one-dimensional case near half-filling[8]:

$$\varepsilon_{\mathbf{k}\pm(\pi/2,\pi/2)} \simeq \pm 2t(k_x + k_y) - \mu + O(tk^3). \qquad (10)$$

The pair $\pm(\pi/2, -\pi/2)$ is characterized by the similar dispersion law

$$\varepsilon_{\mathbf{k}\pm(\pi/2,-\pi/2)} \simeq \pm 2t(k_x - k_y) - \mu + O(tk^3). \qquad (11)$$

The expansions (8)– (11) are valid until $k \lesssim 1$. In its turn, it means that dropping the higher terms of the expansions, one hopes to obtain the correct form of RKKY interaction at $r \gtrsim 1$. Below we revise this statement and compare our analytic results with the numerical findings.

We see that the whole vicinity of the FS can naturally be divided into parts of the mainly two-dimensional hyperbolical and linear character of dispersion. Therefore we can represent the Green's function as a sum of eight different contributions which is symbolically written in the form

$$G(i\omega, \mathbf{r}) = \sum_{\mathbf{k}_0} G_{\mathbf{k}_0}(i\omega, \mathbf{r}) \qquad (12)$$

2

where $\mathbf{k}_0 = \pm(0,\pi), \pm(\pi,0), (\pm\pi/2, \pm\pi/2)$ and *the partial Green's function* $G_{\mathbf{k}_0}(i\omega, \mathbf{r})$ originates from the integration over the part of the Brillouin zone with particular form of dispersion law :

$$G_{\mathbf{k}_0}(i\omega, \mathbf{r}) = \frac{v_0}{(2\pi)^2} \int_{k \lesssim 1} d^2\mathbf{k} \frac{\exp(i(\mathbf{k}+\mathbf{k}_0)\mathbf{r})}{i\omega - \varepsilon_{\mathbf{k}+\mathbf{k}_0}}. \quad (13)$$

It should be noted that this decomposition is a general one and may be done in all cases when the FS possesses the saddle points and flat parts. Hence our consideration of the nearly nested FS may be regarded as a particular example of the analysis of the RKKY interaction for the strongly non-spherical FS.

III. THE GREEN'S FUNCTION FROM THE SADDLE POINTS IN THE SPECTRUM

In this Section we consider the contribution to the Green's function from the vicinities of the saddle points of the spectrum only. The flat parts are analyzed in Section V. As we will show below the saddle points determine the RKKY interaction almost at all directions in r−space except the regions near the diagonals $x = \pm y$ where the contribution from the flat parts of the FS becomes important.

At the first step we use the following auxiliary representation of the Green's function :

$$G(i\omega, \mathbf{r}) = \frac{e^{-i\alpha}}{(2\pi)^2} \int\limits_0^\infty d\tau \int d^2\mathbf{k} \exp\big[i\mathbf{k}\mathbf{r} + \tau e^{i\alpha}\left[i\omega - \varepsilon_k\right]\big]$$

$$(14)$$

where we put $\alpha = sign(\omega)\pi/2$. It is evident that $e^{i\alpha} = i\,sign(\omega)$ but this formal trick facilitates the following analysis of the complex-valued expressions.

The evaluation of the saddle point contribution to the Green's funciton can be made in more general form applicable for the parts of the electronic spectrum near the so-called stationary points[5]. By definition these are the points $\mathbf{k}_0$ where $\varepsilon_{\mathbf{k}}$ is well approximated by the expression

$$\varepsilon_{\mathbf{k}_0+\mathbf{k}} \simeq \frac{1}{2}\mathbf{k}\,\overset{\leftrightarrow}{\mathrm{m}}^{-1}\mathbf{k} - \mu, \quad (15)$$

with the generally anisotropic tensor of masses $\overset{\leftrightarrow}{\mathrm{m}}$ and some effective chemical potential μ. We assume the applicability of (15) for the wave-vectors $\mathbf{k}$ not exceeding some scale κ, comparable to inverse lattice parameter. In other words the significant parts of the FS may be approximately mapped by (15).

In view of (15) the integration over $\mathbf{k}$ in (14) becomes Gaussian one and is easily performed. The only complication here comparing to the case of free electron gas[4] is the finite value of κ which restricts the validity of the

subsequent equations by $r \gtrsim \kappa^{-1}$; we discuss it in more detail below.

Thus we obtain the following expression for the partial contribution to Green's function from the vicinity of $\mathbf{k}_0$

$$G_{\mathbf{k}0}(i\omega, \mathbf{r}) = -e^{-i\alpha} \frac{\sqrt{|det\,\overset{\leftrightarrow}{\mathrm{m}}|}}{2\pi} e^{i\mathbf{k}_0\mathbf{r}}$$

$$\times \int_0^\infty \frac{d\tau}{\tau} \exp[\tau z e^{i\alpha} - \frac{\rho}{2\tau} e^{-i\alpha}] \quad (16)$$

where $z = \mu + i\omega$ and $\rho = \mathbf{r}\,\overset{\leftrightarrow}{\mathrm{m}}\,\mathbf{r}$ is the square of distance *in the metrics defined by the mass tensor*. The last integral is expressed via the modified Bessel (Macdonald) function,[9] namely

$$G_{\mathbf{k}0}(i\omega, \mathbf{r}) = -e^{-i\alpha} \frac{\sqrt{|det\,\overset{\leftrightarrow}{\mathrm{m}}|}}{\pi} e^{i\mathbf{k}_0\mathbf{r}} K_0(\sqrt{-2z\rho}) \quad (17)$$

In the equation (17) the branch of $\sqrt{-2z\rho}$ is chosen from the condition of its positive real part. In particular case of $2\mu\rho > 0$, this latter condition means that the argument of Macdonald function $K_0(\sqrt{-2z\rho})$ has a discontinuity at $\omega = 0$,[9]

$$K_0(\sqrt{-2z\rho}) = \begin{cases} \frac{\pi i}{2} H_0^{(1)}(\sqrt{2\mu\rho}), & \omega/\mu \to +0 \\ -\frac{\pi i}{2} H_0^{(2)}(\sqrt{2\mu\rho}), & \omega/\mu \to -0 \end{cases} \quad (18)$$

where $H_0^{(1,2)}(x)$ are Hankel functions. Note that in the case of spherical Fermi surface the condition $2\mu\rho \equiv k_F^2 r^2 > 0$ is fulfilled automatically. For the electronic type of dispersion $\overset{\leftrightarrow}{\mathrm{m}} > 0$ and $\mu > 0$ while for the hole-like dispersion law one has $\overset{\leftrightarrow}{\mathrm{m}} < 0$ and $\mu < 0$. It is clear from Eq.(18) that for non-spherical Fermi surface the effective Fermi momentum is given by $\sqrt{2\mu\rho} = k_F^* r$ and may strongly depend on the direction in real space (cf. Eq.(26) below).

Let us discuss now the region of applicability of the expression (17). The Gaussian integration in (14) for $\varepsilon_{\mathbf{k}}$ given by (15) is justified upon two conditions. First, the center of quadratic form in $\mathbf{k}$ which is $\tau^{-1}\mathbf{r}\,\overset{\leftrightarrow}{\mathrm{m}}$ should lie within the circle of radius κ, where the expansion (15) is applicable. Second, one should demand the criterion $\tau|\kappa\,\overset{\leftrightarrow}{\mathrm{m}}^{-1}\kappa| \gg 1$ to be satisfied , to ensure the Gaussian value (16). In the principal axes j of $\overset{\leftrightarrow}{\mathrm{m}}$ these criteria can be combined as follows :

$$\tau \gg \max\left[\frac{|r_j m_j|}{\kappa}, \frac{|m_j|}{\kappa^2}\right] \quad (19)$$

At this point our analysis is somewhat different for the cases $k_F^* r = \sqrt{2\mu\rho} \gg 1$ and $k_F^* r \lesssim 1$.

In the first case of largest r the principal contribution to the integral (16) is delivered by $\tau = \tau_0(1 + O(1/\sqrt{2z\rho}))$ with $\tau_0 = \sqrt{\rho/2z} = k_F^* r/(2\mu)$[10]. Simple arguments show then that for the ellipsoidal FS the criterion (19) is always fulfilled, coinciding with the obvious demand $k_F^* \ll \kappa$. For the spectrum with the saddle point the condition (19) may be violated at large distances and near the nodes

$\rho \simeq 0$. Let the angle φ be measured from the $\hat{x}$-axis in $\mathbf{r}$-plane. Then k_F^* is given by (26) and we lose the applicability of (17) at

$$\frac{\sqrt{|t/\mu|}}{r} \ll \sqrt{|\varphi \pm \pi/4|} \lesssim \frac{\sqrt{|\mu/t|}}{a}, \qquad (20)$$

i.e. within a narrow sector along the diagonals if $r/a \gg |t/\mu| \gg 1$.

In the case of $k_F^* r \lesssim 1$ it is the region $|\rho| \lesssim \tau \lesssim |z|$ which is essential in (16). Substituting the lower boundary $\tau = |\rho|$ into (19) we come to the evident condition $\kappa r > 1$ for the ellipsoidal FS. For the FS with the saddle point the criterion (19) is again violated near the node of ρ. For our particular form of the spectrum the Eq.(17) is applicable outside the band along the diagonals $x = \pm y$:

$$r|\varphi \pm \pi/4| > \kappa^{-1} \sim a. \qquad (21)$$

We depict the above regions of applicability on the Figure 1.

Let us now consider the particular form of the Green's functions arising in the case of the tight-binding spectrum (7).

The integration over $\mathbf{k}$ being restricted to the first Brillouin zone leads to the additional phase factor in (17) as discussed in Appendix A. The desired expressions acquire the form :

$$G_{(0,\pi)}(i\omega, \mathbf{r}) = -\frac{i\,sign(\omega)}{2\pi t} K_0(\sqrt{-2z\rho}) e^{i\pi|y|sign(\omega)} \quad (22)$$

$$G_{(\pi,0)}(i\omega, \mathbf{r}) = -\frac{i\,sign(\omega)}{2\pi t} K_0(\sqrt{2z\rho}) e^{i\pi|x|sign(\omega)} \qquad (23)$$

where $\rho = (x^2 - y^2)/2t$ and $\sqrt{|det\,\overleftrightarrow{m}|}$ is replaced by its actual value $1/2t$.

IV. EVALUATION OF THE RKKY INTERACTION

A. integer values of r

We note that if the values of coordinates x, y in (22), (23) coincide with the integer numbers of lattice periods then one has $e^{i\pi|x|sign(\omega)} = e^{i\pi x}$, $e^{i\pi|y|sign(\omega)} = e^{i\pi y}$ and $e^{2i\pi x} = e^{2i\pi y} = 1$. We consider this simpler case first, while the case of non-integer x, y is discussed in the next subsection.

Away from the diagonals $x = \pm y$ in $\mathbf{r}$-space, we have from (4) the following expression :

$$\chi(\mathbf{r}) = \frac{1}{4\pi^2 t^2} \int_{\mu-i\infty}^{\mu+i\infty} \frac{dz}{2\pi i} \Big[K_0^2(\sqrt{-2z\rho}) + K_0^2(\sqrt{2z\rho})$$
$$+ 2e^{i\pi(x+y)} K_0(\sqrt{-2z\rho}) K_0(\sqrt{2z\rho}) \Big] \qquad (24)$$

Here we redefined the variable of integration $\omega \to z = \mu + i\omega$.

As we discussed above if $\mu\rho > 0$ then the function $K_0(\sqrt{-2z\rho})$ has the discontinuity (18) at $z = \mu$. On the contrary the second term in (24) is continuous function of z in this case and the corresponding integral is zero, because one can shift the integration contour to $z \to +\infty$ wherein $K_0(z) \propto e^{-z}$.

At $\mu\rho < 0$ the situation is reversed, hence one can combine these two cases and cast the contribution of first two terms in (24) into the form[11]

$$\chi_1(\mathbf{r}) = \frac{|\mu|}{8\pi t^2} \Phi_1(k_F^* r) \qquad (25a)$$

$$\Phi_1(a) = J_0(a)Y_0(a) + J_1(a)Y_1(a) \qquad (25b)$$

with Bessel functions $J_n(x)$ and $Y_n(x)$ and the direction-dependent value of the effective Fermi momentum

$$k_F^* = \frac{\sqrt{|2\mu\rho|}}{r} = \frac{1}{a}\sqrt{\left|\frac{\mu}{t}\cos(2\varphi)\right|}. \qquad (26)$$

where we restored in the rhs the lattice parameter a. Note that the expression (25) gives the RKKY interaction for the cylindrical Fermi surface as well, in which case k_F^* coincides with the conventional Fermi momentum[4]. The only difference is in the general minus sign resulted from the sign-indefinite property of the mass tensor, $det(\overleftrightarrow{m}) = -1/(4t^2) < 0$.

The asymptotes of this part of RKKY interaction under criteria (20) and (21) are as follows

$$\chi_1(\mathbf{r}) = \frac{|\mu|}{8\pi^2 t^2} \frac{\sin(2k_F^* r)}{(k_F^* r)^2}, \quad k_F^* r \gg 1 \qquad (27a)$$

$$= \frac{|\mu|}{4\pi^2 t^2} \ln k_F^* r, \quad k_F^* r \ll 1 \qquad (27b)$$

Therefore in the limit of large distances the power-law decrease of $\chi_1(\mathbf{r})$ is accompanied by oscillations with the direction-dependent period $2k_F^*$, in accordance with usual expectations, while for the small $k_F^* r$ these oscillations are replaced by logarithmic singularity.

The third term in (24) is the integral of the product of the Green's functions resulting from the regions of the FS with the different character of dispersion. As a result, one has the additional prefactor of the form $\exp(i\mathbf{Q_0 r}) = (-1)^{x+y}$ (for integer x, y). The appearing "antiferromagnetic" wave-vector $\mathbf{Q_0} = (\pi, \pi)$ merely connects two regions in the Brillouin zone, where the dispersion is close to the Fermi level. In this third term of Eq. (24) the discontinuity at $z = \mu$ exists for both signs of $\mu\rho$. The integration over z can also be done[11] and we obtain after some calculations :

$$\chi_2(\mathbf{r}) = e^{i\mathbf{Q_0 r}} \frac{|\mu|}{4\pi^2 t^2} \Phi_2(k_F^* r) \qquad (28a)$$

$$\Phi_2(a) = \frac{J_0(a)K_1(a) - J_1(a)K_0(a)}{a} \qquad (28b)$$

4

The asymptotes of this expression are

$$\chi_2(\mathbf{r}) = e^{i\mathbf{Q}_0\mathbf{r}}\frac{|\mu|\sqrt{2}}{4\pi^2 t^2}\frac{\cos(k_F^* r)}{(k_F^* r)^2}e^{-k_F^* r}, \quad k_F^* r \gg 1 \quad (29a)$$

$$= e^{i\mathbf{Q}_0\mathbf{r}}\frac{|\mu|}{4\pi^2 t^2}\frac{1}{(k_F^* r)^2}, \quad k_F^* r \ll 1 \quad (29b)$$

Let us discuss the significance of this second part of RKKY interaction. First, one sees from (27), (29) that in the far asymptotic region $k_F^* r \gg 1$ the first term $\chi_1(\mathbf{r})$ dominates while $\chi_2(\mathbf{r})$ is exponentially small. In particular, it explains why the $\chi_2(\mathbf{r})$ term could not be obtained by the previous methods[2] — the RKKY interaction as expressed in Ref.[2] was a series in powers of $1/r$, and the exponential tail was evidently missing.

On the contrary, the term $\chi_2(\mathbf{r})$ starts to play a decisive role at smaller distances $k_F^* r \lesssim 1$, where it prevails according to (27), (29). We stress that the condition $k_F^* r > 1$ was essential for the previous theories, while our expressions are applicable at weaker conditions (20),(21). Therefore the part $\chi_2(\mathbf{r})$ represents the *intermediate asymptote* of the RKKY interaction in the nearly-nested situation.

Second we note that $\chi_2(\mathbf{r})$ has the antiferromagnetic sign-reversal character. This feature of the RKKY interaction at short distances appears to be quite general. One can show for other types of dispersion[12] that this kind of short range oscillations is always determined by the wavevector connecting saddle points in the band structure.

To clarify these two items further we consider the case of the perfect nesting of the electronic spectrum, $\mu = 0$, when the far asymptotic regime is not realized. We immediately see the disappearance of the first part of the RKKY interaction (25), while only this term could be obtained in the former methods of $1/r$ expansion. At the same time our second part of RKKY interaction (28) survives. As a result we have

$$\chi(\mathbf{r}) = e^{i\mathbf{Q}_0\mathbf{r}}\frac{1}{4\pi^2 t\,|x^2 - y^2|} \quad (30)$$

This behavior indicates the log-squared singularity of the polarization operator on the antiferromagnetic wave vector $\mathbf{Q}_0$ discussed, e.g., by Dzyaloshinskii[13].

To validate our analytical findings (25), (28) we performed the direct numerical calculation of the RKKY interaction on the square $|x|, |y| \leq 10$ with the spectrum given by (7). The results for $\mu = 0.1$ and $t = 0.5$ are shown on the Figure 2. We plotted on the Figure 2a the calculated value of the RKKY interaction versus the "distance" in the saddle point metrics, $r^* = \sqrt{|x^2 - y^2|}$. According to this convention $k_F^* r = (k_F^*)_{max} r^*$, so we can show the results for the whole plane in a simplest manner; for the chosen parameters $(k_F^*)_{max} = \sqrt{\mu/t} \simeq 0.45$. On the same plot we have drawn the curves $\chi_1(k_F^* r) - \chi_2(k_F^* r)$ and $\chi_1(k_F^* r) + \chi_2(k_F^* r)$, which are the predicted values of the interaction for the odd and even sites, respectively. No additional parameters were used.

We see the remarkable agreement between the calculated points and the theoretical formulas. As we expected at large distances the oscillations in the RKKY are observed while at smaller distances $r^* < \sqrt{t/\mu} \simeq 2.5$ the situation is changed. The interaction for the "odd" sites $x + y = 2n + 1$ (i.e. for $\mathbf{r} = (0,1), (1,2), (0,3)\dots$) is of the antiferromagnetic (negative) sign. The interaction for the "even" sites ($\mathbf{r} = (0,2), (1,3), (0,4)$ *etc.*) has a tendency to be ferromagnetic. In both cases the calculated points closely follow our curves $\chi_1(\mathbf{r}) \pm \chi_2(\mathbf{r})$ up to the interatomic distances. The RKKY interaction expected from the previously known expressions (the term $\chi_1(k_F^* r)$) is shown by a dashed line.

To clearer represent the region of larger r^* we multiplied the calculated points $\chi(\mathbf{r})$ onto the appropriate values of $(r^*)^2$. The same was done for the theoretical curves, the results are shown on the Figure 2b. We see again that at large r^* the interaction is characterized by the usually discussed asymptotic oscillations (27). At the same time the difference between the "odd" and "even" sites is clear at the lower distances.

Note that $\chi(\mathbf{r})$ for the diagonal $x = \pm y$ is not present on the Fig. 2 and cannot be in principle compared to (25), (28) due to the criteria (20), (21); we discuss it also in the next Section.

B. noninteger values of R

Let us now extend our analysis for the case of noninteger values of x, y. One can easily note that now the factors of the type $\exp[i\pi|x|sign(\omega)]$ in (22), (23), (A3) produce another source of discontinuity at $\omega = 0$, in addition to the previously discussed one of the value $\sqrt{2\rho(\mu + i\omega)}$. In particular both first and second terms in (24) acquire the factors $e^{\pm 2i\pi|x|} \neq 1$ and $e^{\pm 2i\pi|y|} \neq 1$, respectively. Therefore both these terms now contribute although in a different manner.

Consider first the case of $|x| > |y|$ and $\mu < 0$, which means $\rho\mu < 0$ and the closed character of the FS. A straightforward calculation[11] shows then that the above expressions (25), (28) are generalized as follows :

$$\chi_1(\mathbf{r}) = \frac{|\mu|}{8\pi t^2}\Big[\cos(2\pi|x|)\Phi_1(k_F^* r)$$
$$+ \sin(2\pi|x|)\Phi_3^{(1)}(k_F^* r) \quad (31a)$$
$$+ \sin(2\pi|y|)\Phi_3^{(2)}(k_F^* r)\Big]$$

$$\chi_2(\mathbf{r}) = \frac{|\mu|}{4\pi^2 t^2}\Big[\cos(\pi|x| + \pi|y|)\Phi_2(k_F^* r)$$
$$+ \sin(\pi|x| + \pi|y|)\Phi_4(k_F^* r)\Big] \quad (31b)$$

with the functions

$$\Phi_3^{(1)}(a) = \frac{1}{2}[Y_0^2(a) - J_0^2(a) + Y_1^2(a) - J_1^2(a)] \quad (32a)$$

$$\Phi_3^{(2)}(a) = \frac{2}{\pi^2}[K_0^2(a) - K_1^2(a)] \quad (32b)$$

$$\Phi_4(a) = \frac{Y_0(a)K_1(a) - Y_1(a)K_0(a)}{a} \qquad (32c)$$

The different terms appeared in (31) have different significance at large and small $k_F^* r$.

In the far asymptotic regime $k_F^* r \gtrsim 1$ the terms $\Phi_3^{(2)}, \Phi_2, \Phi_4$ are exponentially small and we find :

$$\chi(\mathbf{r}) \propto \frac{\sin(2\pi|x| - 2k_F^* r)}{(k_F^* r)^2}, \quad k_F^* r \gtrsim 1 \qquad (33)$$

The period of oscillation in the above expression corresponds to the notion of the calipering points on the FS.[2] We remind that these are the points where the direction of normal to the Fermi surface is (anti)parallel to the direction of $\mathbf{r}$. In other words, the normal to the FS coincides with the direction of the Fermi velocity $\mathbf{v} = (v_x, v_y)$ and it is parallel to $\mathbf{r} = r(\cos\varphi, \sin\varphi)$ provided

$$v_x \sin\varphi = v_y \cos\varphi. \qquad (34)$$

Near the saddle points $(\pm\pi, 0)$ one has $v_x/v_y = -k_x/k_y$ and $k_x^2 - k_y^2 = -\mu/t$. Therefore the calipering points, satisfying the condition (34), are given by $\widetilde{\mathbf{k}}^c = \pm(\cos\varphi, -\sin\varphi)[-(t/\mu)\cos 2\varphi]^{-1/2}$ near the points $(\mp\pi, 0)$, respectively. We measured the wave-vectors from the saddle points, therefore the true caliper of the fermi surface is given by the vector $\mathbf{k}^c = (2\pi, 0) - 2\widetilde{\mathbf{k}}^c$. The scalar product $\mathbf{k}^c \mathbf{r}$ is exactly what one finds in the Eq.(33) since $\widetilde{\mathbf{k}}^c \mathbf{r} = r\sqrt{-\mu\cos(2\varphi)/t} \equiv k_F^* r$.

At the smaller distances $k_F^* r \leq 1$ these are the terms $\Phi_3^{(1)}, \Phi_3^{(2)}, \Phi_2$, which determine the main contribution to $\chi(\mathbf{r})$. In this case one obtains :

$$\chi(\mathbf{r}) \simeq \frac{\pi\cos(\pi|x| + \pi|y|) + \sin 2\pi|x| - \sin 2\pi|y|}{4\pi^3 t|x^2 - y^2|}, \qquad (35)$$
$$k_F^* r \lesssim 1$$

We see again that the interaction has a commensurate period of oscillations, although the oscillations for non-integer $\mathbf{r}$ are not described by a unique factor as it was in Eqs.(29b), (33).

V. THE FLAT PARTS OF THE SPECTRUM

Let us discuss here the contribution to the RKKY interaction produced by the flat parts of the spectrum (11). First we observe that the formalism developed in the main part of the paper cannot be applied to the vicinities of the points $(\pm\pi/2, \pm\pi/2)$ since all the components of the mass tensor are infinite at these points. This very special case should be treated separately; one can also distinguish here the regions of intermediate and far asymptotes. At the intermediate distances $r \lesssim |t/\mu|$ we obtain the Green's function from the vicinities of $(\pi/2, \pi/2)$ and $(-\pi/2, -\pi/2)$ in the form

$$G_{(\pi/2,\pi/2)}(i\omega, \mathbf{r}) = \frac{e^{-i\alpha}}{2t}\delta_\kappa(x - y)\exp\left[i|x|(\pi + z/2t)sign(\omega)\right] \qquad (36)$$

and the corresponding Green's function from the vicinities of $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$ is obtained from this expression by the replacement $y \to -y$. The function $\delta_\kappa(x)$ in (36) has the $\delta-$function-like properties and is defined by

$$\delta_\kappa(x) = \frac{\sin\kappa x}{\pi x}, \quad \kappa \sim \frac{1}{a} \qquad (37)$$

We wish to point out that the power-law decrease of $\delta_\kappa(x)$ at large x stems from our assumption that the absence of dispersion along x is lost abruptly at $|k_x| > \kappa$. In fact the expression (37) is the Fourier transform of $\theta(\kappa - |k_x|)$. In general the dependence of dispersion on k_x is much smoother ; as a result, the decay of $\delta_\kappa(x)$ at large x should be much faster, while the $\delta-$function-like property preserves.

We see that the above Green's function has a sizeable values only in a band $|x - y| \lesssim 1$. Outside this domain the principal contribution to the total $G(i\omega, \mathbf{r})$ (12) is delivered by $G_{(0,\pi)}(i\omega, \mathbf{r})$ and $G_{(\pi,0)}(i\omega, \mathbf{r})$, Eqs. (22) and (23). Particularly it means (see Fig.1) that the terms of the type $G_{(\pi/2,\pi/2)}G_{(0,\pi)}$ in the expression (24) should not be considered.

As a result the contributions to the RKKY interaction from the flat parts of FS acquire the following form :

$$\chi_{flat}(\mathbf{r}) = \frac{\cos x(2\pi + \mu/t)}{4\pi t|x|}\left[\delta_\kappa^2(x - y) + \delta_\kappa^2(x + y)\right], \quad (38)$$
$$|x|, |y| \lesssim |t/\mu|$$

here two terms in the square brackets correspond to the different regions in the $\mathbf{r}$-space. We see that this part of interaction which is present along the diagonals is slowly decaying as $1/r$. The amplitude of it, according to (37) has the model cutoff parameter κ^2. Hence we cannot directly compare this part of RKKY with the results of our numerical calculations, although the overall $1/r$ dependence of RKKY interaction along the diagonals and slow oscillations are verified by the numerical data as well. At small integer values of $x = y$ the RKKY term (38) corresponds to the ferromagnetic sign of the interaction between the localized moments. This behavior however does not define the particular type of magnetic ordering and it is the term (30) which determines it.

At extremely large distances close to diagonal $r \gg |t/\mu|$ the dropped k^3-terms in the expansions (10), (11) become important. Hence the spectrum becomes essentially two-dimensional, with the corresponding change in the character of RKKY. Near the diagonals $\varphi = \pm\pi/4 + \phi$ one has :

$$\chi_{flat}(\mathbf{r}) = -\frac{\sin|x|(2\pi + \mu/t(1 - \phi^2/\phi_0^2))}{4\pi^2|\mu|x^2[1 + \phi^2/\phi_0^2]}, \quad |x| \gg \frac{t}{|\mu|} \qquad (39)$$

This far asymptote of RKKY interaction from the flat parts of dispersion holds in the narrow sectors near the diagonals $|\phi| \lesssim \phi_0 = \sqrt{2}|\mu/4t|$, (cf. (20), (21) and Fig. 1). It has the $1/r^2$ dependence while its period of oscillations correponds to the notion of calipering points discussed above.

VI. CONCLUDING REMARKS

It is worthwhile to compare our expressions for the Green's function with previous results. It was observed (see e.g.[14]) that for the tight-binding spectrum (7) one can use the recurrence relations to express the value of $G(\omega, \mathbf{r})$ in terms of $G(\omega, 0)$. It was noted also however that using these relations one meets the numerical instabilities at large r. Alternatively $G(\omega, \mathbf{r})$ can be estimated at large r by the steepest descent method. The solution obtained by this latter method corresponds to the asymptotes of Eqs. (17), (18) for the case of large $\sqrt{2\mu\rho} = k_F^* r$. In this sense our expressions extend the previous findings for the Green's function and provide the analytical formulas in the region of the intermediate distances $1 \lesssim r \lesssim 1/k_F^*$.

Let us briefly discuss here the role of finite temperatures for our treatment. In this case instead of the integral (24) one considers the sum over the Matsubara frequencies (4) with the Green's functions given by (22), (23). With the use of analytical continuation, this sum can be represented as the integral over the real axis of ω. One can note however directly from the form of the Green's functions that the effect of finite temperatures is important when T exceeds the effective chemical potential μ. At large distances $r \gtrsim \xi = (k_F^*)^{-1}\sqrt{\mu/T} \propto \sqrt{t/T}$ we have the RKKY interaction exponentially suppressed.[15] The opposite case $r \lesssim \xi$ corresponds essentially to the case $\mu = 0$ described by the Eq.(30). Therefore the far asymptote of RKKY leading to possible incommensurate magnetic ordering is absent in this case and we remain with the only tendency to commensurate AF order.

In conclusion we found the closed analytic expressions for the RKKY interaction in a layered metal with nearly nested Fermi surface. Along with the usual $2k_F$-oscillations realized at far distances we demonstrate the existence of the intermediate asymptote of the interaction. This latter asymptote has the commensurate AF type of oscillations and is the only term surviving at the exact nesting. We show that our analytical formulas are in the good accordance with the numerically found values of interaction in a range up to near interatomic distances.

ACKNOWLEDGMENTS

APPENDIX A: THE STATIONARY POINT AT THE ZONE BOUNDARY

Let us consider the case of the stationary point lying on the boundary of the Brillouin zone. We discuss it on the example of the sum of the points $(\pi, 0)$ and $(-\pi, 0)$ for the tight-binding form of dispersion (7). The integration over k_y meets no difficulties, while the domains of integration over k_x, namely $(-\pi, -\pi + \kappa)$ and $(\pi - \kappa, \pi)$, could be combined as follows :

$$
\begin{aligned}
G_{ZB}(i\omega, x) &= e^{-i\pi x} \int_0^{\kappa} \frac{dk_x}{2\pi} \exp\left[ik_x x - \tau e^{i\alpha}\frac{k_x^2}{2m_x}\right] \\
&\quad + (x \to -x) \\
&= A\left[\cos(\pi x)\mathrm{Erf}\left(\frac{k\gamma}{2} - i\frac{x}{\gamma}\right)\Big|_{k=-\kappa}^{\kappa}\right. \\
&\quad \left. + 2i\sin(\pi x)\,\mathrm{Erf}\left(-i\frac{x}{\gamma}\right)\right]
\end{aligned} \tag{A1}
$$

with

$$
A = \frac{1}{\pi\gamma}\exp\left[-e^{-i\alpha}\frac{m_x x^2}{2\tau}\right], \tag{A2}
$$

$$
\gamma = \sqrt{e^{i\alpha}\frac{2\tau}{m_x}}, \quad Re(\gamma) > 0.
$$

The demand for the argument $\pm\kappa\gamma/2 - ix/\gamma$ in (A1) to be large corresponds to the criteria of applicability of our expressions (20), (21) and we do not discuss it here. Similar to the above treatment at $k_F^* r \gg 1$ one has $\tau \simeq k_F^* r/(2\mu)$ and $|x/\gamma| \geq k_F^* r \gg 1$. At $k_F^* r \lesssim 1$ we saw that $|\rho| \lesssim \tau \lesssim |z|$; on the other hand the values of $|z|$ at which the integral (24) saturated were of order of $1/|\rho|$. Therefore we can let $\tau \sim |\rho|$ and obtain $|x/\gamma| \sim \sqrt{|x^2 m_x/\rho|} \geq 1$. Hence in both cases the argument of the second error function in (A1) is large enough, while its sign coincides with the sign of a product $-x\omega m_x$. Therefore the Green's function has a following form :

$$
G_{zb}(i\omega, x) = \sqrt{\pi}A\exp[-i\pi|x|sign(\omega m_x)] \tag{A3}
$$

This result means that the Gaussian value of integral is attained in one of the above domains of integration. Note that $G_{zb}(i\omega, x)$ is an even function of x ; it is a manifestation of the reflecting property of the Brillouin zone boundary[5]. For a particular choice of our spectrum (9) we have $m_x = -1/2t < 0$ and thus the formula (23).

[1] M.A. Ruderman, C. Kittel, Phys.Rev. **96**, 99 (1954); T. Kasuya, Progr.Theoret.Phys. (Kyoto) **16**, 45 (1956); K. Yosida, Phys.Rev. **106**, 893 (1957).

[2] L.M. Roth, H.J. Zeiger, T.A. Kaplan, Phys.Rev. **149**, 519 (1966).

[3] M. van Schilfgaarde *et al.*, Phys.Rev.Letters **74**, 4063 (1995) and references therein.

[4] D.N. Aristov, Phys. Rev. B **55**, 8064 (1997).

[5] A.A.Abrikosov,*Fundamentals of the theory of metals*, North-Holland, Amsterdam (1988).

[6] V.I. Belinicher and A.L. Chernyshev, Phys.Rev. B**49**, 9746 (1994) and references therein.

[7] see e.g. E.Dagotto, Rev. Mod. Phys., **66**, 763, (1994).

[8] A.Luther, Phys.Rev. B**50**, 11446 (1994).

[9] I.S. Gradshtein, I.W. Ryzhik, *Tables of Integrals, Series and Products*, (Academic, New York, 1965).

[10] Note that one can neglect the $\omega-$dependence of τ here since the subsequent integration over ω in (24) saturates over $\omega \lesssim \mu/(k_F^* r) \ll \mu$.

[11] *Handbook of Mathematical Functions*, eds. M. Abramowitz and I.A. Stegun, (Natl. Bureau of Standards, New York, 1964).

[12] D.N. Aristov, to be published.

[13] I.E. Dzyaloshinskii, Sov. Phys. JETP **66**, 848 (1987).

[14] E.N. Economou, *Green's Functions in Quantum Physics*, 2nd edition (Springer–Verlag, New York, 1990).

[15] Note that for spherical FS one would have $T \ll \mu$ and the temperature correlation length $\xi \propto \mu/T$
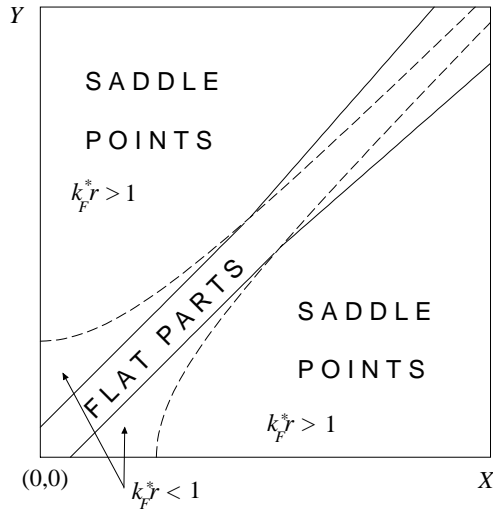
FIG. 1. The regions of applicability of the different Green's functions in the sector $x > 0$, $y > 0$ of the **r**-space. The contributions from the saddle points of the spectrum are given by (22), (23) and are defined away from the diagonal. The expression (36) provides the contribution from the flat parts of dispersion. The solid line is the border between the applicability regions of corresponding equations. At the same plot the curve $k_F^* r = 1$ is shown by the dashed line.
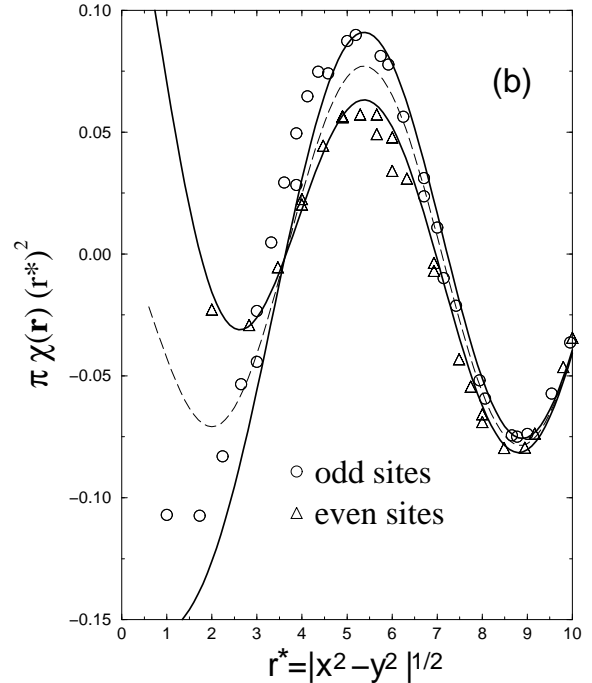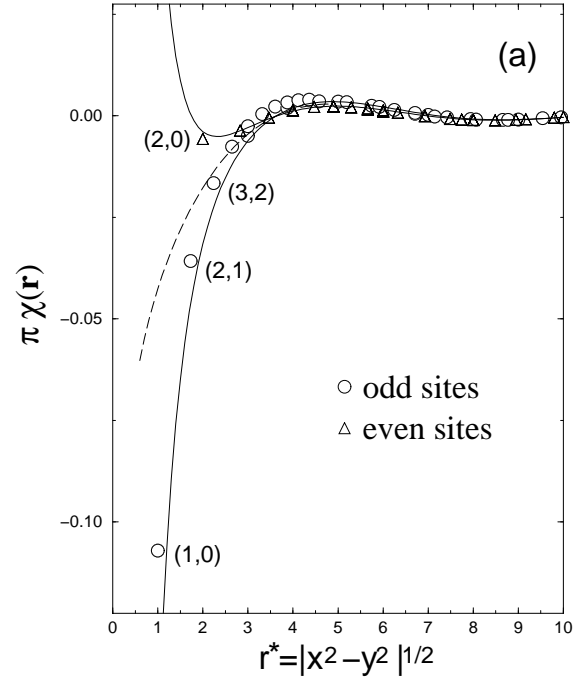
FIG. 2.   a) The calculated RKKY interaction for the tight-binding spectrum (7) with $\mu = 0.1, t = 0.5$ is shown along with the theoretically obtained curves. b) The same quantity plotted in a modified way, for clearer representation of the region of larger r^*. The actual coordinates of some sites are indicated. One can note the remarkable accordance between the numerical findings and the analytical results in the intermediate region, where the curves for "odd" and "even" sites differ visibly. The asymptotic solution for RKKY extended to shorter distances is shown by a dashed line for comparison.